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Lattice Boltzmann Methods for Compressible Two-Phase Flow Problems

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Abstract. By a combination of well-established mathematical techniques, it is possible to construct a general numerical method for solving any hyperbolic system of conservation laws with the following interesting features: time-explicit, unconditionally stable, accepting unstructured arbitrary meshes, of arbitrary order and naturally parallel. We give an overview of the construction of the method and an example of application to a multiphase compressible flow sedimentation problem.

VECTORIAL KINETIC REPRESENTATION OF CONSERVATION LAWS

Conservation laws in fluid mechanics

Most of the inviscid models in fluid mechanics can be expressed by conservation laws of the form

$$\partial_t \mathbf{w} + \sum_{k=1}^{D} \partial_k \mathbf{q}^k(\mathbf{w}) = 0, \tag{1}$$

where D is the space dimension, $\mathbf{x} \in \mathbb{R}^D$ is the space variable and $t \in [0,T]$ the time variable. The unknown is the vector of conservative variables $\mathbf{w}(\mathbf{x},t) \in \mathbb{R}^m$. The model is entirely given by the physical conservative flux: $\mathbf{q}(\mathbf{w})\cdot\mathbf{n} = \sum_{k=1}^{D} \mathbf{q}^k(\mathbf{w}) n_k$. For instance, in this work we consider the following two-phase flow model with the conservative variables

$$\mathbf{w} = (\rho, \rho\mathbf{u}^T, \rho\varphi)^T, \tag{2}$$

where ρ is the density, $\mathbf{u}$ the velocity and φ the mass fraction of the first phase. The flux is given by

$$\mathbf{q}(\mathbf{w})\cdot\mathbf{n} = \begin{pmatrix} \rho\mathbf{u}\cdot\mathbf{n} \\ \rho(\mathbf{u}\cdot\mathbf{n})\mathbf{u} + p\mathbf{n} \\ \rho\varphi\mathbf{u}\cdot\mathbf{n} \end{pmatrix}. \tag{3}$$

The pressure p is a given function of ρ and φ (see [1] for more details).

The model is mathematically stable under an hyperbolicity condition: $\mathbf{A}(\mathbf{w},\mathbf{n}) = D_{\mathbf{w}} q(\mathbf{w})\cdot\mathbf{n}$ must have real eigenvalues λ_i, $i = 1 \dots m$. It is well-known that such models can have very complex features, such as shock waves, turbulent behaviour, *etc.* In addition, the numerical simulation is difficult. For instance, standard numerical methods are constrained by a stability condition of the form $\Delta t \leq \beta \Delta x / \lambda_{\max}$, where $\lambda_{\max} = \max_i |\lambda_i|$, Δt is the time discretisation parameter, Δx the space discretisation parameter and β is the Courant–Friedrichs–Lewy (CFL) constant of the numerical method. Other issues are related to numerical accuracy, long time behaviour, numerical oscillations, for instance.

Jin-Xin over-relaxation

In this section we present the method for a space dimension $D = 1$. We thus consider the hyperbolic system:

$$\partial_t \mathbf{w} + \partial_x \mathbf{q}(\mathbf{w}) = 0. \tag{4}$$

This system can be approximated by the Jin-Xin over-relaxation technique [2, 3]. It consists in introducing an additional artificial variable $\mathbf{z}$, the approximated flux, and to solve

$$\partial_t \mathbf{w} + \partial_x \mathbf{z} = \mathbf{0}, \tag{5}$$

$$\partial_t \mathbf{z} + \lambda^2 \partial_x \mathbf{w} = \boldsymbol{\mu}, \tag{6}$$

where $\lambda > 0$ is a constant given parameter. The choice of the source term $\boldsymbol{\mu}$ is very important. It is generally defined as a relaxation source term, but for a rigorous formulation, we prefer the following definition. We first introduce the Dirac comb:

$$\Psi(t) = \sum_{i \in \mathbb{Z}} \delta(t - i\Delta t), \tag{7}$$

where δ is the Dirac measure, and then take

$$\boldsymbol{\mu}(x,t) = \theta \Psi(t) \left(\mathbf{q}(\mathbf{w}(x,t)) - \mathbf{z}(x,t^-) \right), \quad \theta \in [1,2]. \tag{8}$$

In other words, at times $t = i\Delta t$, $\mathbf{z}$ has jumps in time and:

$$\mathbf{z}(x,t^+) = \theta \mathbf{q}(\mathbf{w}(x,t)) + (1-\theta)\mathbf{z}(x,t^-). \tag{9}$$

If the relaxation parameter $\theta = 1$, we recover the standard Jin-Xin first order splitting. In the Jin-Xin scheme, each step of duration Δt is made of two substeps:

- Free transport step: one solves (5)-(6) with $\mu = 0$. This is very easy because the equation is then linear with constant coefficient. On a regular grid, when $\Delta x = \lambda \Delta t$, it can even be solved exactly. This is the main idea at the base of the Lattice-Boltzmann Method (LBM) [4].
- Relaxation step: during the free transport step, the approximate flux $\mathbf{z}$ has deviated from the exact one $\mathbf{q}(\mathbf{w})$. The relaxation consists simply in resetting $\mathbf{z}$ to $\mathbf{q}(\mathbf{w})$.

Let us note that the scheme is explicit and unconditionally stable if λ is large enough (sub-characteristic condition [5]). But it is only first order. The **over-relaxation** corresponds to $\theta = 2$. It leads to a second order method in time [6].

Kinetic interpretation

The Jin-Xin scheme can be reinterpreted as a kinetic scheme with Boltzmann-like interpretation. Indeed, we can diagonalise the linear hyperbolic operator. For this, consider the change of variables

$$\mathbf{k}^+ = \frac{\mathbf{w}}{2} + \frac{\mathbf{z}}{2\lambda}, \quad \mathbf{k}^- = \frac{\mathbf{w}}{2} - \frac{\mathbf{z}}{2\lambda}. \tag{10}$$

$$\mathbf{w} = \mathbf{k}^+ + \mathbf{k}^-, \quad \mathbf{z} = \lambda \mathbf{k}^+ - \lambda \mathbf{k}^-. \tag{11}$$

Then, the kinetic quantities $\mathbf{k}^+$ and $\mathbf{k}^-$ satisfy the following transport equations at velocities $\pm\lambda$:

$$\partial_t \mathbf{k}^+ + \lambda \partial_x \mathbf{k}^+ = \mathbf{r}^+, \quad \partial_t \mathbf{k}^- - \lambda \partial_x \mathbf{k}^- = \mathbf{r}^-, \tag{12}$$

where

$$\mathbf{r}^\pm(x,t) = \theta \Psi(t) \left(\mathbf{k}^{eq,\pm}(\mathbf{w}(x,t^-)) - \mathbf{k}^\pm(x,t^-) \right) \tag{13}$$

and the "Maxwellian" states $\mathbf{k}^{eq,\pm}$ are given by

$$\mathbf{k}^{eq,\pm}(\mathbf{w}) = \frac{\mathbf{w}}{2} \pm \frac{\mathbf{q}(\mathbf{w})}{2\lambda}. \tag{14}$$

Formally, we see that the kinetic variables $\mathbf{k}^+$ and $\mathbf{k}^-$ satisfy free transport equations at velocity $\pm\lambda$, with relaxation to "Maxwellian" equilibrium at each time step.

EQUIVALENT EQUATION AND BOUNDARY CONDITIONS

The kinetic approach amounts to introducing new artificial variables to the original system in order to simplify its numerical resolution. This leads to some difficulties for handling the boundary conditions correctly on these artificial variables. In addition, it is not clear to understand in which sense system (5)-(6) is an approximation of (4). We have provided in [3] a rigorous analysis of the equivalent equation of the over-relaxation system in the second order case ($\theta = 2$). For presenting this analysis, let us introduce the "flux error"

$$\mathbf{y} := \mathbf{z} - \mathbf{q}(\mathbf{w}). \tag{15}$$

From (9), we see that at time $t = i\Delta t$

$$\mathbf{y}(x,t^+) = -\mathbf{y}(x,t^-). \tag{16}$$

Therefore $\mathbf{y}$ oscillates around 0 at a frequency $1/\Delta t$. For the analysis, it is thus better to consider the solution only at even (or only at odd) times steps $t = 2i\Delta t$, like in a stroboscope. We can prove the following result:

Theorem: if the solution of the over-relaxation ($\theta = 2$) scheme (5), (6), (8) is considered at even time steps, then, up to $O(\Delta t^2)$ second order terms in Δt, its equivalent equation in $(\mathbf{w},\mathbf{y})$ is the following hyperbolic system of size $2m$:

$$\partial_t \mathbf{w} + \partial_x \mathbf{q}(\mathbf{w}) = 0, \tag{17}$$

$$\partial_t \mathbf{y} - \mathbf{q}'(\mathbf{w})\partial_x \mathbf{y} = 0. \tag{18}$$

Remarks:

- The conservative vector $\mathbf{w}$ satisfies the expected conservative system at order $O(\Delta t^2)$.
- The flux error $\mathbf{y}$ satisfies a very simple non-conservative equation. In the analysis, there is no mathematical assumption on the smallness of $\mathbf{y}$ at the initial time, even if for physical reasons we expect $\mathbf{y}$ to be small.
- The waves for $\mathbf{w}$ and $\mathbf{y}$ move in opposite directions. In practice, this means that one always has to impose m boundary conditions at a boundary, independently of the supersonic or subsonic nature of the flow. This can lead to great simplifications in the numerical methods.
- From the analysis of the third order terms, it is possible, in simple cases, to also recover the subcharacteristic stability condition $\lambda < \lambda_{\max}$ (see [3]) .

This analysis allows us to construct schemes that are second order, even at the boundaries [3].

EXTENSION TO HIGHER DIMENSIONS

The above formalism can be extended to arbitrary dimension [7]. A rigorous and very nice entropy analysis of the general method also exists [8]. This analysis ensures the robustness of the schemes built with this approach. The extension to higher dimension is obtained through a generalised Maxwell-Boltzmann kinetic methodology. First, we consider vectorial kinetic equations of the form

$$\partial_t \mathbf{k} + \sum_{k=1}^{D} \mathbf{V}^k \partial_k \mathbf{k} = \theta \Psi(t) \left(\mathbf{k}^{eq}(\mathbf{w}(\mathbf{x},t^-)) - \mathbf{k}(\mathbf{x},t^-) \right), \tag{19}$$

where $\mathbf{k}(\mathbf{x},t) \in \mathbb{R}^n$, $\mathbf{x} \in \mathbb{R}^D$ and the matrices $\mathbf{V}^k$, $1 \le k \le D$ are **diagonal** and **constant**. The conservative variables $\mathbf{w}$ are deduced from the kinetic data $\mathbf{k}$ by the formula $\mathbf{w} = \mathbf{P}\mathbf{k}$ where $\mathbf{P}$ is a constant $m \times n$ matrix, $m < n$. The equilibrium ("Maxwellian") distribution $\mathbf{k}^{eq}(\mathbf{w})$ is a given function of $\mathbf{w}$ that satisfies $\mathbf{P}\mathbf{k}^{eq}(\mathbf{w}) = \mathbf{w}$.

Multiplying (19) on the left by $\mathbf{P}$ we formally see that when $\Delta t \to 0$, we obtain an approximation of

$$\partial_t \mathbf{w} + \sum_{k=1}^{D} \partial_k \mathbf{q}^k(\mathbf{w}) = 0, \tag{20}$$

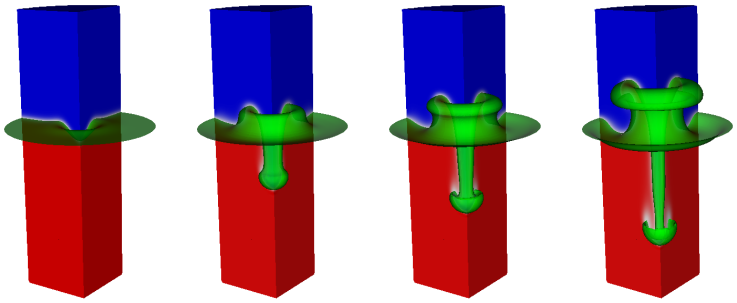

FIGURE 1. Compressible sedimentation test case. A heavy phase (in blue) is initially over the light phase (in red). The interface is represented in green. We observe the growth of the Rayleigh-Taylor instability at several times.

where the flux is given by

$$\mathbf{q}^k(\mathbf{w}) = \mathbf{P}\mathbf{V}^k\mathbf{k}^{eq}(\mathbf{w}). \tag{21}$$

By a proper choice of $\mathbf{V}$ and $\mathbf{k}^{eq}$, it is possible to recover any flux $\mathbf{q}(\mathbf{w})$ and this choice is not unique. This formalism contains the above 1D formalism but also many more. For instance, the classical LBM can be put in this framework [1].

APPLICATION TO COMPRESSIBLE SEDIMENTATION

We have applied the above method for solving several physical problems represented by hyperbolic conservation laws. An important point is that in practice the numerical method amounts to only solving transport equation at **constant** kinetic velocities $\mathbf{V}$, which are not related to the physical velocity $\mathbf{u}$. Solving constant-velocity transport is very easy on a structured grid: the solution is explicit and exact. This the base of the LBM scheme. When the grid is unstructured, the resolution is a little bit more difficult, if one wants to respect the physical conservation property. We have chosen to do it with an upwind Discontinuous Galerkin method. With this choice, it is possible to construct a very high order **explicit** scheme that is **unconditionally stable**, independently of the size of the time step Δt. The algorithm is based on the "downwind numbering" algorithm. Details and more references are given in [1]. On Fig. 1 we reproduce the results of a sedimentation test case. The two-phase model is given by (2)-(3) with an additional gravity source term. A heavy blue phase is initially placed over a light red phase. We observe the growth of a Rayleigh-Taylor instability. The mesh is unstructured. Only one quarter of the flow is represented. The important point is that the computations have been performed in a stable way with a CFL number $\beta = 10$. More practical details can be found in [1].

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